MCCI and Ducted Fuel Injection (Part 2)

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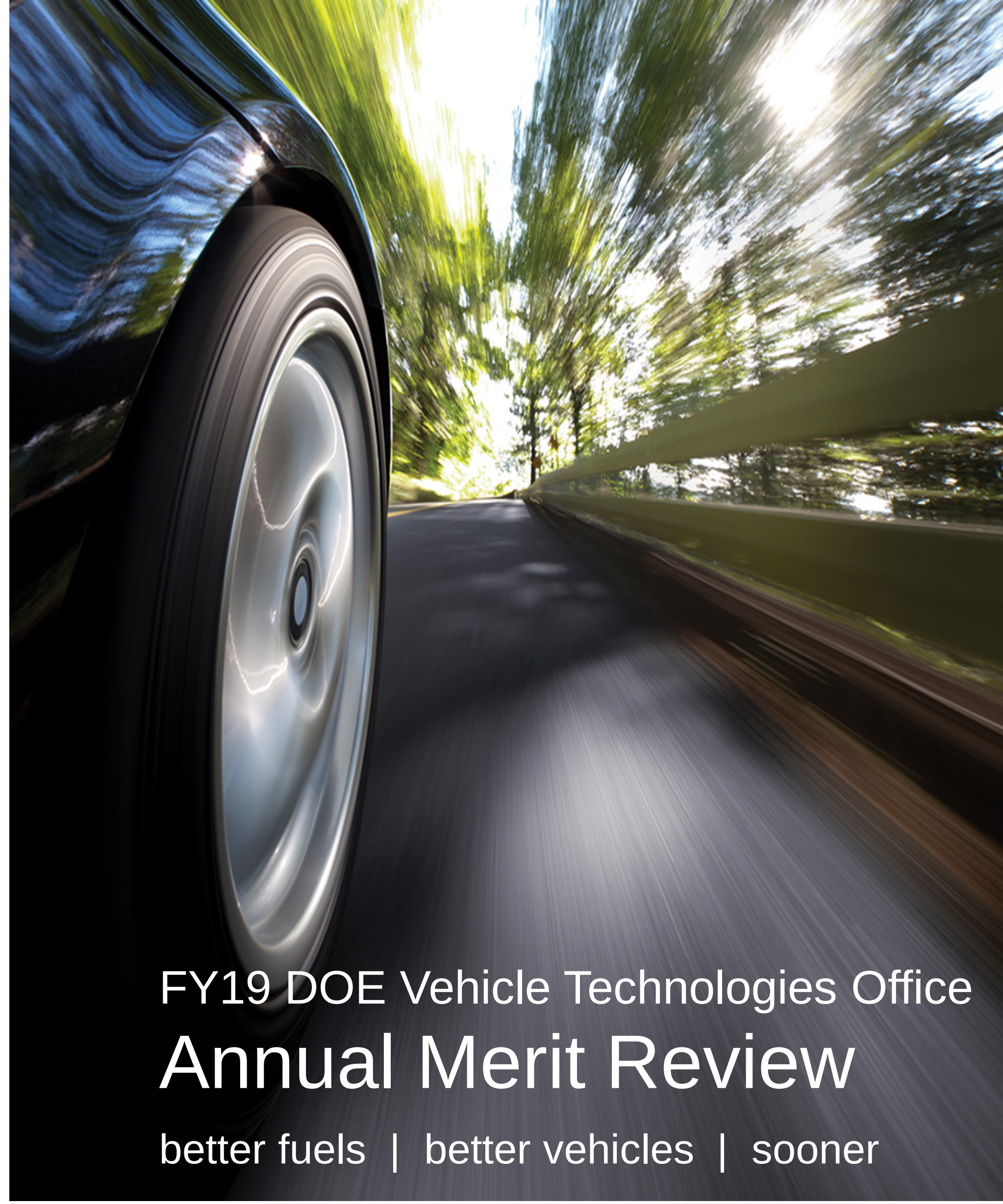
Project # FT078



Co-Optimization of Fuels & Engines

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

Overview

Four Projects

E.2.2.8 - Catalyst light-off and cold-start emissions (Wissink)
E.2.2.9 - Catalyst heating operation (Busch)
G.2.18 - Effect of Fuel Properties on In-nozzle Cavitation (Som)
E.1.4.1 - X-ray Measurements of Injection and Mixture Formation (Powell)

Timeline

- All projects new in FY2019
- Projects end after FY2021

Budget

- CN and Cold Start: $222k
- Oxy Fuels and Cold Start: $160k
- Cavitation Modeling: $120k
- Cavitation Measurements: $155k

Collaboration

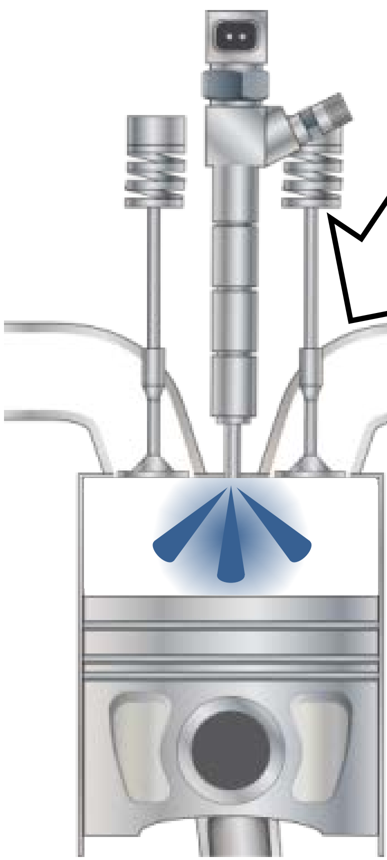
- Catalysts: Ford, Daimler
- Cavitation: Powell, Som, Pickett, ECN, Co-Optima Fuels Team

Barriers

- Understand and improve combustion during cold start to reduce emissions
- Provide a comprehensive understanding of fuel sprays with support from advanced diagnostics and high-fidelity modeling tools
- A comprehensive understanding of fuel sprays, combustion, and emissions formation is needed to develop optimal combustion system designs

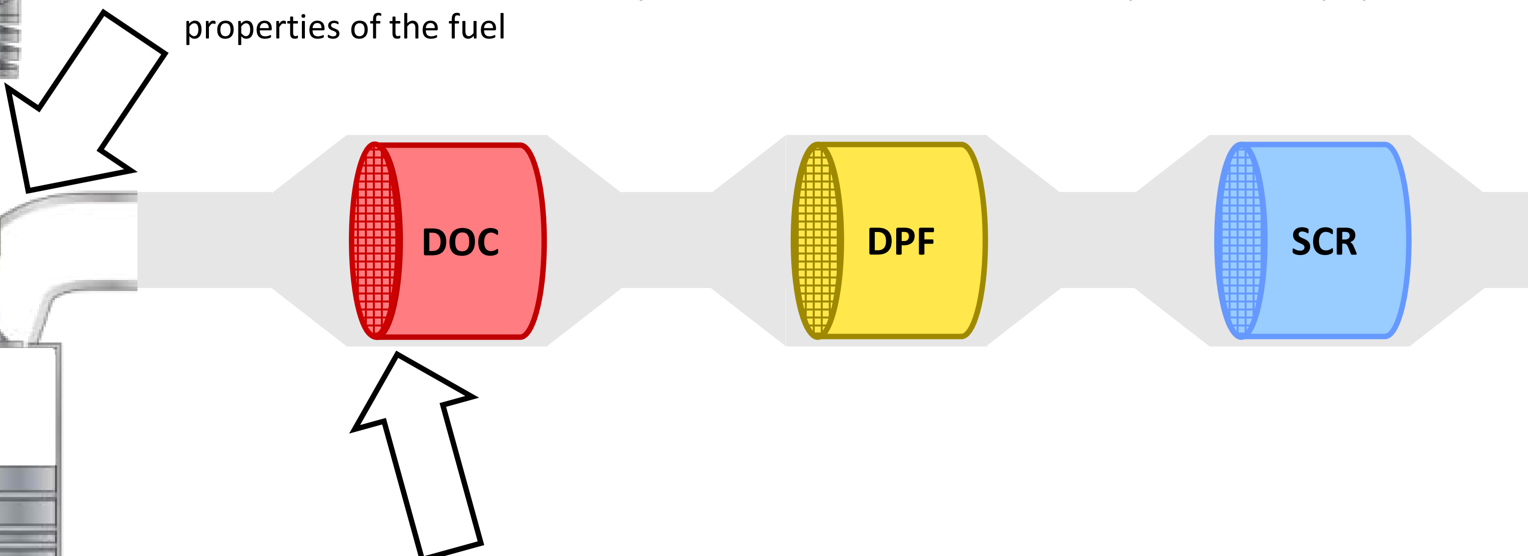
Relevance: The Big Picture

Develop a fundamental understanding of the relationship between fuel properties and emissions



In-Cylinder Emissions Reduction (sprays, mixture formation)

- Cavitation Modeling, Cavitation Measurements
- Cavitation and erosion alter injection and combustion , and depend on the physical properties of the fuel



In-Cylinder Effects on Emissions Control (catalyst heating, cold start)

- CN and Cold Start, Oxy Fuels and Cold Start
- Fuel properties impact combustion, emissions, and aftertreatment performance

Relevance

- **In-cylinder emissions reduction** requires detailed knowledge of fuel effects on injection and mixture formation
  - **Objective**: Perform nozzle flow measurements and simulations to characterize the influence of critical fuel properties on cavitation. Identify fuel properties that increase cavitation and erosion.
  - **Impact**: Improved fundamental understanding of cavitation and erosion. Integrate a new cavitation erosion model into a computational screening tool for new fuels.

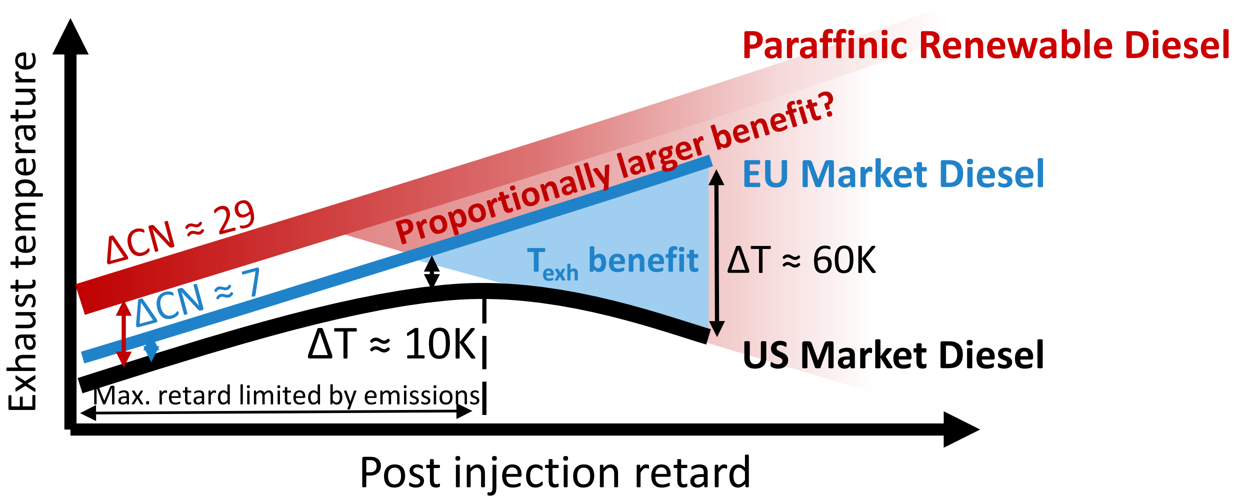
- **Decreasing emissions at cold start** requires either decreased engine-out emissions, or faster catalyst light-off
  - **Objective**: Assess the ability of cetane number to increase exhaust temperature
  - **Objective**: Assess the ability of oxygenated fuels to lower HC emissions
  - **Impact**: Improved understanding of how fuel properties can be manipulated in order to decrease emissions under cold start conditions

Milestones

Month / Year	Description of Milestone or Go/No-Go Decision	Status
March 2019	**Oxy Fuels & Cold Start**: GO/NOGO: Assess infrared in-cylinder imaging technique to detect aldehydes	NOGO: IR signature not detected
March 2019	**Cavitation Modeling:** Differences in cavitation characteristics for different MCCI fuels characterized.	60% complete (awaiting properties for MCCI fuels)
June 2019	**Oxy Fuels & Cold Start:** Complete initial thermodynamic/UHC emissions assessment of three oxygenated blendstocks	On track
June 2019	**CN and Cold Start:** Quantify impact of cetane number on exhaust enthalpy under cold-start conditions for bookend fuels	On track
June 2019	**Cavitation Measurements**: X-ray imaging of cavitation intensity and extent in MCCI nozzles with three fuel blends	On track

Approach – CN, Oxygenates, and Cold Start

- MCCI cold-start strategies use retarded post injection to increase exhaust temperature and quickly reach catalyst light-off – limited by NOx/HC emissions
- Modest increase in cetane number (CN) has been shown[1] to allow increase of exhaust temperature within emissions constraints
- CN approach: explore limits of this strategy with high-CN renewable diesel on a multi-cylinder, heavy-duty MCCI engine platform (ORNL) – directly applicable to new CARB emissions regulations (0.02 g/bhp-hr NOx)
  - Do the benefits of increasing CN continue proportionally or reach point of diminishing return?
  - Can further increases in exhaust temperature be made without increasing NOx/HC emissions?
  - Does high-CN fuel with late post create any unburned or partially-oxidized species that affect catalyst performance?
- Oxygenate approach: thermal, emissions, and optical measurements in a single-cylinder swirl-supported diesel engine (SNL) using three different oxygenate blends with certification diesel
  - Are oxygenated blendstocks able to decrease pollutant emissions for a given exhaust temperature or enable later post injection combustion phasing?



[1]Kurtz, E. and Polonowski, C., "The Influence of Fuel Cetane Number on Catalyst Light-Off Operation in a Modern Diesel Engine," SAE Int. J. Fuels Lubr. 10(3):2017, https://doi.org/10.4271/2017-01-9378.

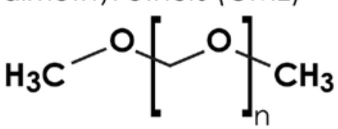
Accomplishments: CN and Cold Start

- Engine platform and experimental hardware selected
  - Multi-cylinder Detroit DD15, 139 mm bore size representative of segment
  - Open ECU architecture: full control of common rail and injections
  - Instrumented cylinder head for combustion analysis
  - FID for total HC emissions, FTIR for detailed speciation
- Fuels have been selected and acquired
  - Low CN fuel: US 2007 Certification Diesel
    - ~46 CN, 178-337 °C boiling range
  - High CN fuel: Paraffinic Renewable Diesel
    - ~75 CN, 189-309 °C boiling range
- Facilities upgrade required to maintain cold-start conditions specified by ACEC Tech Team (20 °C coolant and oil)
  - Chiller has been specified and requisitioned
  - Facilities expected to be fully operational in April
- On track to perform experiments to quantify impact of cetane number on exhaust enthalpy under cold-start conditions in FY19

Accomplishments: Oxy Fuels and Cold Start

- Thermodynamic and exhaust HC emissions measurements have been completed for post injection timing sweeps with three oxygenated blends:
  - OME blend, dibutyl ether, and 1-octanol splash blended with cert diesel
- Oxygenated additives can significantly reduce total hydrocarbon emissions
  - Ethers do this more effectively than 1-octanol
- Oxygenated additives affect the ignition and combustion of the pilot and main injections, but the impact on the post combustion depends on post injection timing
  - The combustion of late post injections is not significantly affected by post injection timing
  - Preliminary evidence: changing fuel composition may not promote robust ignition of late posts

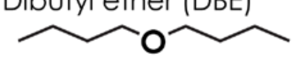
Polyoxymethylene dimethyl ethers (OME)



CN: 77.5

OME blend: n≈3-5

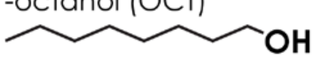
Dibutyl ether (DBE)



$C_8H_{18}O$

CN: ~105

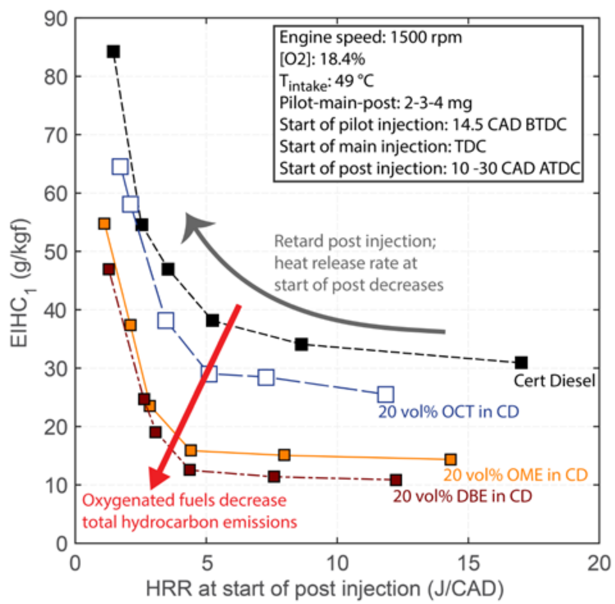
1-octanol (OCT)

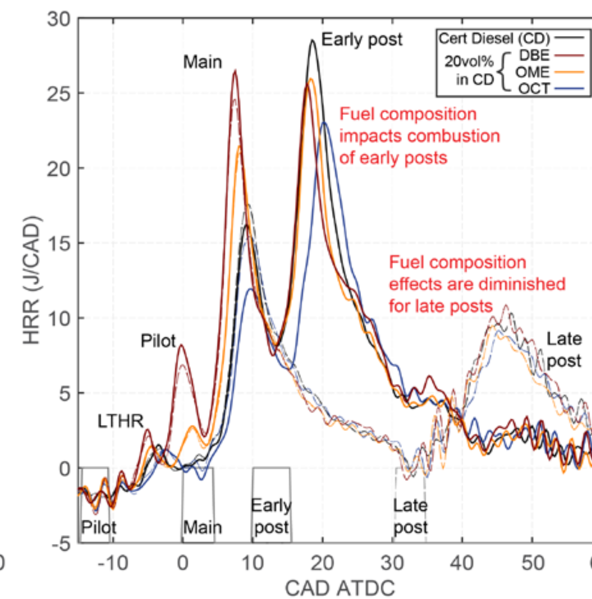


$C_8H_{18}O$

CN: 37

Cert diesel CN: 43.9

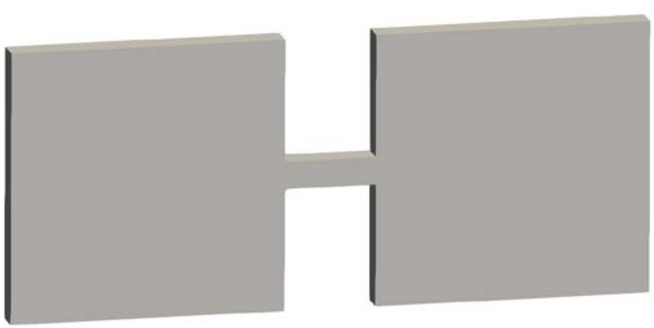


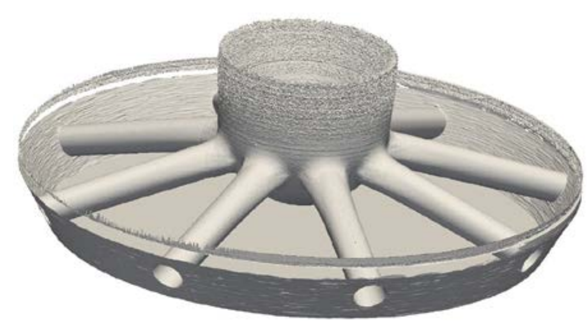


Approach: Cavitation Modeling

- Fuel property effects on cavitation and erosion are tested using a suite of techniques with varying levels of fidelity and complexity
  - Erosion propensity and severity assessed using model developed at Argonne within the DOE Core Program[1] and validated for single pure fuel[2]
  - Local sensitivity analysis used to identify influential fluid properties
  - Pure fuels of interest tested in geometries of varying complexity:

Throttle → **Research Grade Injector : ECN Spray C** → **Commercial Multi-hole Injector**



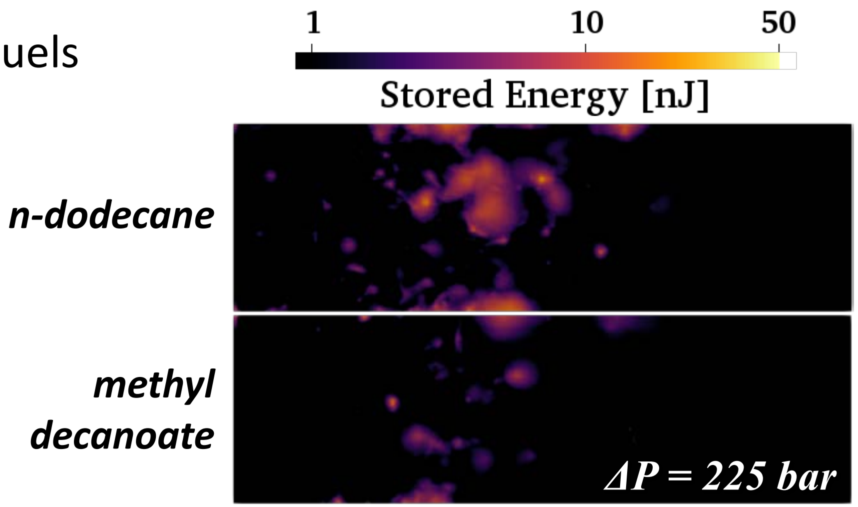


1. S. Som AMR Presentation: acs075_som_2018
2. Magnotti et al., ICLASS 2018.

Accomplishment: Cavitation Modeling

Erosion Propensity has been Predicted for Several Fuels

- Simulations in the throttle geometry were used as an initial fuel screening tool to assess their relative cavitation and erosion propensity
- Comparison of MCCI and SI fuels with baseline fuels:
    - n-dodecane
    - hexadecane
    - methyl decanoate (MD)
    - undecane
    - iso-octane
    - ethanol
- Variance-based sensitivity analysis[1] of cavitation and erosion predictions to selected liquid fuel properties revealed strong dependencies on liquid density and dynamic viscosity, respectively
- For pure fuels, the predicted erosion severity ranking was found to be negatively correlated with the liquid dynamic viscosity



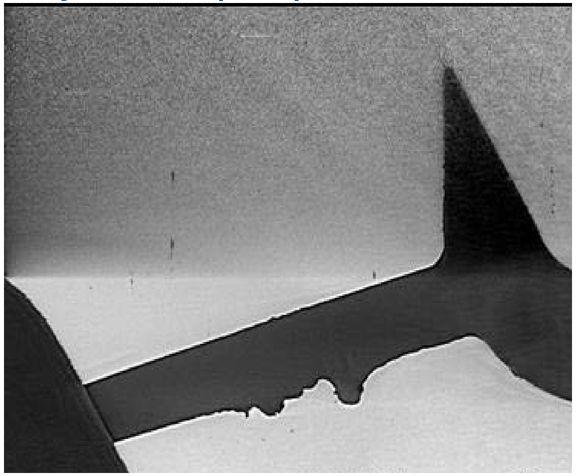
Predicted Erosion Severity Ranking	Fuel	μ = μ(T = 330 K) [Pa-s]
1	iso-octane	3.26E-04
2	n-dodecane	8.52E-04
3	ethanol	6.16E-04
4	undecane	6.99E-04
5	methyl decanoate	1.12E-03
6	hexadecane	1.66E-03

1. Magnotti and Som, ILASS-Americas, 2019.

Approach: Cavitation Measurements

- There is some understanding of how fuel properties (esp. vapor pressure) effect cavitation, but almost no work is available on erosion
- Fuels with lower vapor pressure may lead to more severe erosion
  - Enhanced cavitation
  - Higher intensity pressure waves at bubble collapse
- Two areas of investigation
  - **Measurements of cavitation**: Fundamental measurements of how fuel properties affect cavitation
  - **Measurements of erosion**: Measurements of nozzle erosion and the effect of fuel properties

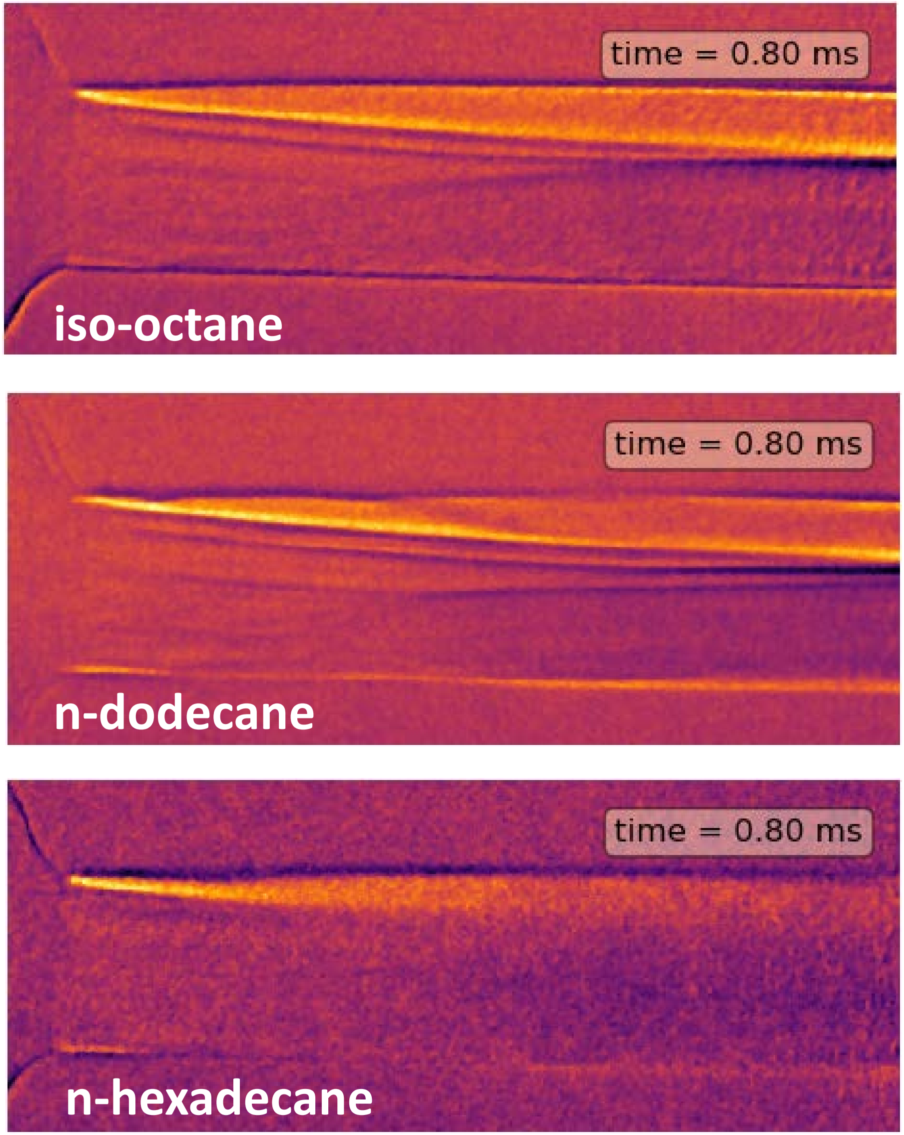
Multi-hole diesel injector eroded by low-vapor-pressure fuel



Tzanetakis *et al*, SAE 2019-01-0263

Accomplishments: Cavitation Measurements

- Recent measurements imaged flow separation in the “Spray C” nozzle
- Studied cavitation intensity and extent for three fuels with a range of vapor pressures
- Flow is similar between iso-octane and n-dodecane.
- Hexadecane shows weaker, less-defined flow separation layer.
  - Lower vapor pressure, higher viscosity
  - Cavitation is more dynamic
  - Dynamics may impact fuel spray distribution, combustion
- Fuel effects on cavitation measured under realistic conditions for the first time



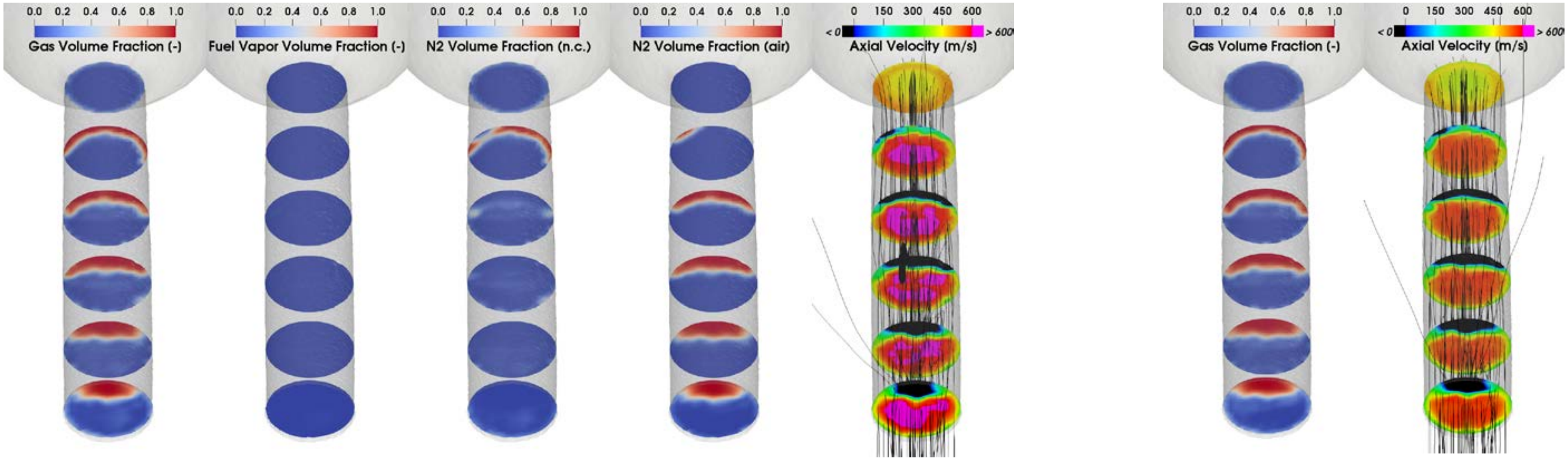
P_{inj} = 1500 bar, P_{amb} = 20 bar

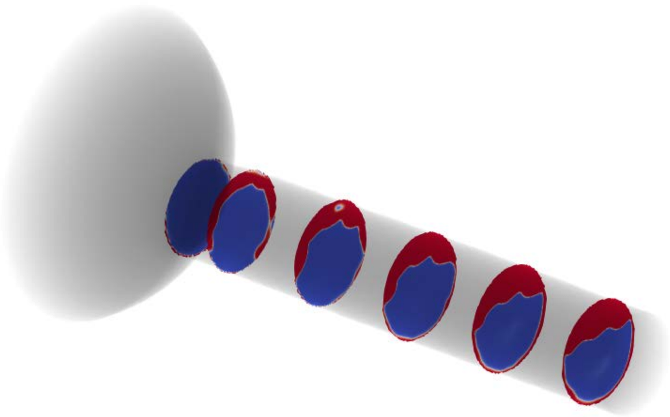
Accomplishment: Cavitation Modeling & Expt

Measurements and Predictions of Show Good Agreement

n-dodecane

Methyl-decanoate





X-ray flow tomography data of **n-dodecane** injection at 1500 bar

Simulations of ECN Spray C showed a Gas Volume Fraction distribution that is comparable to that found in x-ray experiments and can help explaining its nature and composition

LES simulations performed with fixed maximum needle lift

Large velocity and mass flow rate differences (10%) due to different fuel properties

Gas volume fraction is similar at quasi-steady-state flow conditions

Response to Previous Year Reviewers' Comments

All four projects are new in FY 2019, and were not reviewed last year

Collaboration and Coordination with Other Institutions

- **CN and Cold Start**
  - Daimler, Ford: Technical discussions and support
  - Neste: Renewable diesel
- **Oxy Fuels and Cold Start**
  - Ford Motor Company: regular meetings and teleconferences to discuss experimental approach and results
- **Cavitation Simulations**
  - Argonne: Experimental team and Leadership Computing Facility
  - Univ. Central Florida, NREL: fuel physical properties
  - Univ. of Perugia: Collaboration on Spay C simulations
- **Cavitation Measurements**
  - Argonne: Simulations team and Advanced Photon Source
  - Sandia, Engine Combustion Network: Injectors for study, choice of operating conditions, dissemination of results

Remaining Challenges and Barriers

- **CN and Cold Start**
  - Current approach with two “bookend” fuels does not indicate if trend is linear or has antagonistic or synergistic behavior at intermediate CN or fuel blend levels
  - Need to translate impact of exhaust enthalpy and emissions under cold-start conditions to light-off performance of diesel oxidation catalyst
- **Oxy Fuels and Cold Start**
  - Need a mechanistic understanding of how oxygenated components impact mixture formation, ignition, and combustion processes to enable cleaner cold start operation

Cavitation Simulations

  - There is limited availability of experimental data to characterize multiphase flow development and erosion severity for a range of fuels, especially in practical geometries. Collaborating with experimentalists who can provide such data is critical to validating and informing paths towards predictive fuel screening tools
- **Cavitation Measurements**
  - Running injectors for extended erosion tests is not practical at Argonne. Need to find a partner who can assist us with this task.

Proposed Future Research

- **CN and Cold Start**
  - Experiments will use *blends* of the "bookend" fuels, other high-CN fuels to identify non-linearity or diminishing returns in CN trends for exhaust enthalpy and engine-out emissions
  - Use measured exhaust species concentrations as input conditions for bench-flow reactor study of impact of CN and diesel oxidation catalyst light-off performance. Distribute results through CLEERS.
- **Oxy Fuels and Cold Start**
  - In-cylinder high-speed liquid and vapor-phase fuel imaging, natural luminosity imaging to understand oxygenate impacts on mixture formation, ignition, and combustion
- **Cavitation Simulations**
  - Complete simulation of pure fuels in research nozzle, validate with x-ray experiments
  - Extend screening tool to evaluate cavitation, erosion of fuel *blends*, with blending limit guidelines.
  - Evaluate *multi-hole* injectors, increase fidelity using HPC and Argonne-developed best practices
- **Cavitation Measurements**
  - The cavitation simulations group has requested measurements using methyl decanoate because of its predicted low propensity for erosion. Future measurements will attempt to validate this.
  - Measurements of erosion in a canonical nozzle geometry, establishing the link between fuel properties and erosion rates.

Any proposed future work is subject to change based on funding levels

Summary

- **CN and Cold Start**
  - Cetane number (CN) is an important fuel property for MCCI as it can dictate how aggressively the post injections can be retarded for quick catalyst warm-up during cold-start. This task will quantify the effect of high-CN fuel on engine-out exhaust enthalpy and emissions under cold-start conditions.
- **Oxy Fuels and Cold Start**
  - Oxygenated fuels reduce total hydrocarbon emissions in MCCI catalyst heating operation, but further study is needed to understand their impact on the ignition of late post injections
- **Cavitation Simulations**
  - Computational screening tool for pure fuels identified trends relating fuel properties to cavitation, and flagged fuels with increased propensity for cavitation and erosion
- **Cavitation Measurements**
  - Measurements have found variations in cavitation with fuel properties. The measurement results will be shared with the simulations group to validate their work.